High Pressure Behavior of Cubic $ZrMo_2O_8$ *	X17B1

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Negative thermal expansion (NTE) materials are of considerable scientific and technological interest. Their use in composites may facilitate the control of thermal expansion and allow the attainment of zero expansion. The high-pressure behavior of NTE materials is relevant to their application, as the NTE material may experience compression from the surrounding matrix material when used as a filler in a composite. Phase changes that occur under pressure such as that seen in cubic ZrW_2O_8 (transformation to an orthorhombic phase at 2.5 kbar) are undesirable, as the original expansion properties are lost. We have started to investigate the high-pressure behavior of the NTE materials cubic $ZrMo_2O_8$ and cubic $HfMo_2O_8$ *in situ* at X17B1. Experiments were carried out at pressures up to 60 kbar and at temperatures up to 800 °C. The influence of hydrostatic versus non-hydrostatic pressure was also examined using i) a standard boron epoxy cell without a fluid pressure-transmitting medium and ii) a teflon cell with a methanol/ethanol mixture as the pressure-transmitting medium. Non-hydrostatic conditions lead to considerable amorphization at pressures as low as 4-5 kbar, while no structural changes could be seen at the same pressures under hydrostatic conditions. When the amorphous materials were heated under pressure, crystallization to a denser monoclinic polymorph was observed. This polymorph is known to be the thermodynamically stable form of $ZrMo_2O_8$ but had not been seen for $HfMo_2O_8$ prior to this work. * Work supported by grants #'s EAR 89-20239, DMR-9623980, N00014-95-1-1116 from the NSF to SUNYSB; from the NSF and the ONR to Georgia Tech; by the DOE under contract #DE-AC02-98CH10886 to the NSLS; and by the German National Merit Foundation.

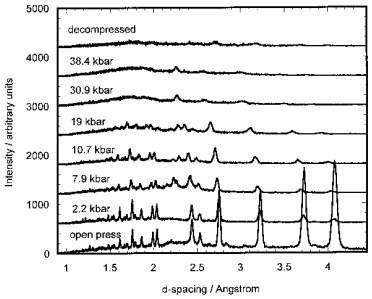

Figure 1. Cubic $ZrMo_2O_8$ in a teflon cell (hydrostatic)

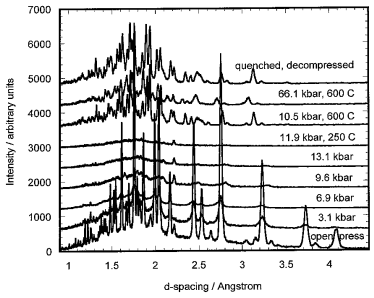

Figure 2. Cubic $ZrMo_2O_8$ in a standard cell (non-hydrostatic)